

ABSTRACT

The invention relates to reference libraries of composite spectra that consolidate, into a single searchable data set, multiple independent spectra taken of a chemical compound under multiple conditions, generally on a single instrument. The reference libraries may be used, for example, to increase the analytical power of mass spectrometers such as API-CID mass spectrometers. The multiple independent spectra are converted into a composite spectrum by performing a number of steps. First, units on the x-axis of at least one, and generally all but one, of the independent spectra are renumbered so that the numerical range of the x-axes of the spectra do not perfectly overlap. Second, the x-axes of the independent spectra are aligned on a composite x-axis. Methods and programs for making and using the reference libraries and devices containing the reference libraries are also disclosed.